

# Light nuclei and hypernuclei from Lattice QCD (A=2,3,4)

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#### Nuclear Physics with Lattice QCD

Quantum Chromodynamics (QCD) is the underlying theory governing the interaction between quarks and gluons, the strong force, and therefore, responsible for all the states of matter in the Universe. Analytical solutions of QCD in the low energy regime cannot be obtained due to the complexity of the quark-gluon dynamics. The only known non-perturbative method that systematically implements QCD from first



institutional NPLQCD effort is to make predictions for the structure and interactions of nuclei using lattice QCD

The mission of the multi-

principles is its formulation on a discretized space-time, lattice QCD. This numerical simulation of the theory consists in a Monte Carlo evaluation of a functional integral. Our goal is to extract information on hadronic interactions, relevant to nuclear processes, through Lattice QCD, using the enormous computing capabilities that the most modern supercomputers offer us, specially on those sectors where experiments are difficult to perform.

NPL OCD info

## Lattice Quantum Chromo Dynamics

space-time lattice  $N_s \times N_s \times N_s \times N_t$ 



(anti) periodic boundary conditions

For numerical calculations in QCD, the theory is formulated on a (Euclidean) space-time lattice, as depicted in the right cartoon.

$$L >> \text{ relevant scales } >> b \quad \left(\frac{1}{L} << m_{\pi} << \Lambda_{\chi} << \frac{1}{b}\right) \qquad \text{Cost} \approx \alpha \left[\frac{1}{m_{q}}\right] \left[V\right]^{a} \left[\frac{1}{b}\right]^{\gamma}$$

finite volume L, discretization (finite spacing) b, value of the light quark masses

#### Brief introduction to the lattice formalism

LQCD is a non-perturbative implementation of Field Theory, which uses the Feynman <u>path-integral approach</u> to evaluate transition matrix elements



the classical path corresponds to the path with the minimum action

in quantum mechanics one sums over all possible paths

evolution of a quantum state (1-D QM)  $\langle x_f, t_f | x_i, t_i \rangle$ 

 $\langle x_f, t_f | x_i, t_i \rangle = \langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle$ 

The quantum propagation is expressed as a weighted sum over paths. The weight is a complex phase factor given by the exponential of i times the classical action *S*.

#### Brief introduction to the lattice formalism



#### Brief introduction to the lattice formalism



The propagation amplitude is re-expressed in terms of the Euclidean action,  $S_E$ 

$$\int_{x(0)=x_i}^{x(t)=x_f} D[x_1, x_2, \dots, x_{N-1}] e^{-\Delta \tau \sum_k \left[\frac{m}{2} \left(\frac{x_{k+1}-x_k}{\Delta t}\right)^2 + V(x_k)\right]}$$

The weight of each path is a real positive quantity, looking like a **Boltzmann factor** 



Real oscillating phase  $\rightarrow$  decaying exponential

Analogy with the partition function of a classical statistical mechanics system

Expectation values:

$$\langle O \rangle = \underbrace{1}_{Z} DUDqD\overline{q}O[q,\overline{q},A] e^{-S_{E}[\overline{q},q,A]}$$

$$\left\langle G[\phi] \right\rangle_{T} = \underbrace{\sum_{\phi} e^{-\frac{E[\phi]}{kT}} G[\phi]}_{\phi} \left( \sum_{\phi} e^{-\frac{E[\phi]}{kT}} \right)$$

~Thermal average over configurations



are taken to satisfy a Grassmann algebra

$$\{\psi,\psi\} = \{\psi,\overline{\psi}\} = \{\overline{\psi},\overline{\psi}\} = 0$$
  
i.e.  $\psi\psi = \overline{\psi}\overline{\psi} = 0$  and  $\psi\overline{\psi} = -\overline{\psi}\psi$ 

QCD partition function in Euclidean space-time

$$Z = \int DA_{\mu} D\overline{\psi} D\psi \exp(-S_{QCD}) = \int DA_{\mu} D\overline{\psi} D\psi \exp\left(-\int d^{4}x \left(\frac{1}{4}G_{\mu\nu}^{a}G_{a}^{\mu\nu} + \sum_{f}\overline{\psi}_{f}[D_{\mu}\gamma_{\mu} + m]\psi_{f}\right)\right)$$

$$matter fields$$

$$i = 1, 2, 3, 4 \quad \text{Dirac index}$$

$$\psi^{iaf}: a = 1, 2, 3 \quad \text{color index}$$

$$f = 1, 2, ... n_{f} \quad \text{flavor index}$$



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$$\left| \left\langle O \right\rangle = \frac{1}{Z} \int DA_{\mu} D\psi \ D\overline{\psi} O[\psi, \overline{\psi}, A] \ e^{-S_{E}[\overline{\psi}, \psi, A]} \right|$$

expectation values

#### Integration over the quark fields

$$Z = \int DA_{\mu} D\overline{\psi} D\psi \exp(-S_{QCD}) = \int DA_{\mu} D\overline{\psi} D\psi \exp\left(-\int d^{4}x \left(\frac{1}{4}G_{\mu\nu}^{a}G_{a}^{\mu\nu} + \sum_{f}\overline{\psi}_{f}[D_{\mu}\gamma_{\mu} + m]\psi_{f}\right)\right)$$
$$Z = \int DA_{\mu} \exp(-S) = \int DA_{\mu} \det\left[M_{f}(A)\right]\exp(-S_{gluon})$$

$$(S = S_{gluon} + S_{f}) \quad \text{very demanding}$$

$$S_{f} = \overline{\psi}M_{f}(A)\psi \quad \det\left[M_{f}(A)\right] \equiv \det\left(\mathcal{D}[A] + m\right) = \prod_{q=1}^{N_{f}} \det\left(\mathcal{D}[A] + m_{q}\right)$$

fermion (quark) matrix nonlocal function of *U* 

When computing expectation values of any given operator *O*, the quark fields in *O* are re-expressed in terms of quark propagators using Wick's Theorem: write all possible contractions for the fields (removing the dependence of quarks as dynamical fields)

$$\left| \left\langle O \right\rangle = \frac{1}{Z} \int DA \, D\psi \, D\overline{\psi} O[\psi, \overline{\psi}, A] \, e^{-S_E[\overline{\psi}, \psi, A]} \right|$$

expectation values

Integration over the quark fields

connected diagrams

disconnected diagrams

# **Correlation functions**

One-hadron correlation function



# **Correlation functions**



#### One-hadron correlation function



one can produce positive/negative (parity) energy states by using the projector:

$$\Gamma_{\pm} = \frac{1}{2} \left( 1 \pm \gamma_0 \right)$$

Masses of (colourless) QCD bound states

 $C(t) = \left\langle 0 \left| \phi(t) \phi^{\dagger}(0) \right| 0 \right\rangle \xrightarrow{\phi(t) = e^{Ht} \phi e^{-Ht}} \left\langle \phi \right| e^{-Ht} \left| \phi \right\rangle$ 

Insert a complete set of energy eigenstates:

$$C(t) = \sum_{n} \langle \phi | e^{-Ht} | n \rangle \langle n | \phi \rangle = \sum_{n} |\langle \phi | n \rangle|^{2} e^{-E_{n}t} \longrightarrow Z_{0} e^{-E_{0}t}$$

i.e. one can obtain the energy of the state provided we see the large time exponential fall-off of the correlation function (Euclidean time evolution suppresses excited states)

average over N gauge-field

configurations  $\{U_{x\mu}\}^i$ 

with i = 1, 2, ... N





mass

Masses of (colourless) QCD bound states



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Insert a complete set of energy eigenstates:

$$C(t) = \sum_{n} \langle \phi | e^{-Ht} | n \rangle \langle n | \phi \rangle = \sum_{n} |\langle \phi | n \rangle|^{2} e^{-E_{n}t} \xrightarrow{t \to \infty} Z_{0} e^{-E_{0}t}$$

The g.s. energy can be more clearly seen by looking at the effective mass plots:

$$\frac{C(t) \sim Z_0 e^{-E_0 t}}{C(t + \delta t) \sim Z_0 e^{-E_0 (t + \delta t)}} \to m_{eff} = \frac{1}{\delta t} \log \frac{C(t)}{C(t + \delta t)}$$
$$\sim -\frac{d}{dt} \log C(t)$$







**HELE**I

baryons: exponential degradation of the signal with time

 $N\sigma^{2}(C) = \langle CC^{\dagger} \rangle - |\langle C \rangle|^{2}$  $\langle C \rangle \sim A_{1} e^{-m_{1}t}$  $\langle CC^{\dagger} \rangle \sim A_{2} e^{-m_{2}t}$ 

pion: 
$$m_1 = m_{\pi}$$
 and  $m_2 = 2m_{\pi}$   
nucleon:  $m_1 = m_N$  and  $m_2 = 3m_{\pi}$ 

A nucleons: 
$$\frac{\langle C \rangle}{\sigma} \sim \sqrt{N} \exp\left\{-A\left(M_N - \frac{3m_{\pi}}{2}\right)t\right\}$$

#### signal-to-noise independent of time

signal-to-noise degradation with time

pion: 
$$\frac{\langle C(t) \rangle}{\sigma(t)} \sim \frac{\sqrt{N}A_0 \ e^{-m_{\pi}t}}{\sqrt{\left(A_2 - A_0^2\right)} \ e^{-m_{\pi}t}} \sim \sqrt{N}$$



nucleon: 
$$\frac{\langle C \rangle}{\sigma} \sim \sqrt{N} \exp\left\{-\left(M_N - \frac{3m_{\pi}}{2}\right)t\right\}$$

#### NPLQCD, Phys.Rev. D84 (2011) 014507



Some current challenges in the extraction of hadron masses:

Optimize the intepolating fiels in order to maximize the weight of a given state

 $\varphi^{s}(\vec{x},t) \equiv \sum_{\vec{y}} f_{s}(\vec{x},\vec{y}) \varphi(\vec{y},t)$ 

different choices for the smearing function: The use of **gaussian smeared operators** optimizes the overlap onto the ground-state hadrons



results obtained with a smeared source and working with point-like and smeared sink



Some current challenges in the extraction of hadron masses:

Develop analysis techniques to extract excited states from the two-point correlators: multiexponential fits, generalize the Effective Mass method to two or more exponential functions (Matrix-Prony), etc.







Two-particle correlators  $\longrightarrow$  Energy of the interacting 2-particle system  $C_{H_{A}H_{B},\Gamma}(\vec{p}_{1},\vec{p}_{2},t) = \sum_{\vec{x}_{1}\vec{x}_{2}} e^{i\vec{p}_{1}\vec{x}_{1}} e^{i\vec{p}_{2}\vec{x}_{2}} \Gamma^{\beta_{1}\beta_{2}}_{\alpha_{1}\alpha_{2}} \langle J_{H_{A},\alpha_{1}}(\vec{x}_{1},t)J_{H_{B},\alpha_{2}}(\vec{x}_{2},t)\overline{J}_{H_{A},\beta_{1}}(x_{0},0)\overline{J}_{H_{B},\beta_{2}}(x_{0},0) \rangle$ spin tensor interpolating operators at large t  $C_{H_{A}H_{B}}(\vec{p},-\vec{p},t) \sim \sum_{n} Z^{(i)}_{n;AB}(\vec{p})Z^{(f)}_{n;AB}(\vec{p})e^{-E^{AB}_{n}(\vec{0})t}$  $m_{\pi} \sim 390$  MeV,  $L_{s} \sim 2.5$  fm



#### LQCD calculations involving A > 2 particles

Greater complexity of multinucleon systems as compared to single meson and baryon calcs

# Wick contractions at que quark level, to form the correlation function is naively  $N_u! N_d! N_s!$ 

$$((A+Z)!(2A-Z)!)$$
 <sup>3</sup>H  $\rightarrow$  2880 <sup>4</sup>He  $\rightarrow$  518400

cheapest 3-baryon system:  $\Xi^0 \Xi^0 n$ , with 3! 2! 4! = 288 Wick contractions





#### How do we get the low-energy scattering parameters and binding energies?

The Maiani-Testa Theorem (*C. Michael, Nucl. Phys. B327(1989; L. Maiani and M. Testa, Phys. Lett. B245, 585 (1990)*) tells us that one cannot extract multi-hadron S-matrix elements from <u>Euclidean space Green functions at infinite volume</u> except for kinematical thresholds.

Scattering amplitudes are in general complex

$$|NN\rangle_{out} = S |NN\rangle_{in} \rightarrow _{out} \langle NN |NN\rangle_{in} = _{in} \langle NN |S|NN\rangle_{in} = e^{i2\delta}$$

below inelastic thresholds

In Euclidean space-time, there is no distinction between in- and out-states. Therefore, the matrix elements one can extract are real numbers, and any signal of the phase due to the interaction is lost.

In non-relativistic Quantum Mechanics, it was known (*K. Huang and C.N. Yang, Phys. Rev.* 105, 767 (1957)) that placing the particles in a finite volume shifts their energies, and these shifts depend on their interactions.

M. Lüscher generalized this results to Quantum Field Theory (*M. Lüscher, Commun. Math. Phys.* 105 153 (1986); *Nucl. Phys.* B354, 531 (1991)): extract the scattering length from the volume dependence of two-particle energy levels at finite volume (up to inelastic thresholds)

#### First, extract the energy-shift due to the interaction:







#### How do we get scattering parameters or binding energies ?

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In the finite volume, below the inelastic thresholds, the energies satisfy the eigenvalue equation:

$$q_{n} \cot \delta(q_{n}) = \lim_{\Lambda_{n} \to \infty} \left\{ \frac{1}{\pi L} \sum_{n}^{\Lambda_{n}} \frac{1}{|\vec{n}|^{2} - \left(\frac{Lq_{n}}{2\pi}\right)^{2}} - \frac{4\Lambda}{L} \right\} = \frac{1}{\pi L} S\left(\frac{q_{n}^{2}L^{2}}{4\pi^{2}}\right) + O(e^{-ML})$$
(3D zeta function)
$$\Delta E_{n}^{(AB)} \equiv \Delta E_{n}^{(AB)}(\vec{0}) \equiv E_{n}^{(AB)}(\vec{0}) - m_{A} - m_{B}$$

$$= \sqrt{q_{n}^{2} + m_{A}^{2}} + \sqrt{q_{n}^{2} + m_{B}^{2}} - m_{A} - m_{B}$$

$$= \frac{(q_{n}^{2})}{2\mu_{AB}} + \dots \text{ lattice extractions}$$

$$q_{n} \cot \delta(q_{n}) = -\frac{1}{a} + \frac{1}{2}r_{0}q_{n}^{2}$$

$$\bullet : \text{ location of the E eigenstates in the finite volume}$$

Beane, Bedaque, Parreño, Savage, Phys. Lett. B585 (2004) 106-114

$$\Delta E_0 = \frac{p^2}{M} = \frac{4\pi a}{ML^3} \left[ 1 - c_1 \frac{a}{L} + c_2 \left(\frac{a}{L}\right)^2 + \dots \right]$$
Ground state energy shift

Recovering M. Lüscher, Commun. Math. Phys. 105, 153 (1986) (L>>a)

$$\Delta E_1 = \frac{4\pi}{ML^2} - \frac{12\tan\delta_0}{ML^2} \Big[ 1 + c'_1 \tan\delta_0 + c'_2 \tan^2\delta_0 \Big] + \dots \quad \text{with} \quad \delta_0 = \delta(p_{E_1})$$

First excited state energy shift





NPLQCD, Phys. Rev. D81 (2010) 054505



NPLQCD, Phys. Rev. D81 (2010) 054505

#### infinite volume extrapolations with enough statistics for (hyper) nuclear systems

Heavier quark masses:

resources required to generate configurations and q-propagators are smaller degradation in the signal-to-noise ratio in multinucleon correlation functions is reduced

#### calculations at the SU(3)-flavor symmetry point

L/b T/b	β	$b m_q$	<i>b</i> (fm)	<i>L</i> (fm)	T (fm)	$m_{\pi}$ (MeV)	$m_{\pi}L$	$m_{\pi}T$	$N_{\rm cfg}$	N <sub>src</sub>
244832484864	6.1 6.1 6.1	$-0.2450 \\ -0.2450 \\ -0.2450$	0.145 0.145 0.145	3.4 4.5 6.7	6.7 6.7 9.0	806.5(0.3)(0)(8.9) 806.9(0.3)(0.5)(8.9) 806.7(0.3)(0)(8.9)	14.3 19.0 28.5	28.5 28.5 38.0	3822 3050 1905	96 72 54

NPLQCD, PRD 87, 034506 (2013); PRC 88, 024003 (2013)

no physical light-quark masses yet only one lattice spacing

#### Anisotropic lattices: $N_t >> N_s$

(N<sub>f</sub>=2+1 clover-improved Wilson fermion actions)

higher resolution in the time direction:

better study of noisy states better extraction of excited states reduce the systematic due to fitting (confident plateaus)



 $-i \cot(\delta)$ 

1.

0.6

0.2

 $-i \cot(\delta)$ 





#### Nucleon-Nucleon





 $(N_f=2+1, b = 0.09 \text{ fm}, m_p = 0.51 \text{ GeV}, L:2.9 \text{ fm to } 5.8 \text{ fm})$ 

From calculations of the two-nucleons at rest and moving in the lattice volume



L ~ 3.4 fm, 4.5 fm, and 6.7 fm, b ~ 0.145 fm and @  $m_{\pi}{\sim}800~MeV$ 



From calculations of the two-nucleons at rest and moving in the lattice volume



L ~ 3.4 fm, 4.5 fm, and 6.7 fm, b ~ 0.145 fm and @  $m_{\pi}{\sim}800~MeV$ 



Increasing complexity of performing contractions with the number of hadrons

To study the interaction of multi-meson/baryon states, a large number of contractions are required; in fact the number grows factorially with the number of particles involved.

# Wick contractions to form the correlation function is naively  $N_u! N_d! N_s!$ 

The triton (nnp) involves 2880 ( $N_u$ =4 and  $N_d$ =5)

However some careful counting, identifying redundant contractions, can reduce this number to a smaller # of distinct contractions.

Recursive algorithms would be needed to study even the light nuclei. (Detmold & Savage, PRD82 (2010) 014511)



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# Wick contractions to form the correlation function is naively  $N_u! N_d! N_s!$ 

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NPLQCD Phys. Rev. D87 (2013), 034506

flavor-SU(3) symmetry physical strange quark mass (no electromagnetic interactions)

 $A \le 4 \& |s| \le 2$ :

(Quark-hadron contraction method: Detmold & Orginos, PRD87 (2013) 114512)

Label	L/b	T/b	$\boldsymbol{\beta}$	$b m_q$	$b  [{\rm fm}]$	$L [{\rm fm}]$	$T  [{\rm fm}]$	$m_{\pi}  [{ m MeV}]$	$m_\pi \; L$	$m_\pi \ T$	$N_{ m cfg}$	$N_{ m src}$
Α	24	48	6.1	-0.2450	0.145	3.4	6.7	806.5(0.3)(0)(8.9)	14.3	28.5	3822	48
В	32	48	6.1	-0.2450	0.145	4.5	6.7	806.9(0.3)(0.5)(8.9)	19.0	28.5	3050	<b>24</b>
С	48	64	6.1	-0.2450	0.145	6.7	9.0	806.7(0.3)(0)(8.9)	28.5	38.0	1212	32

Isotropic clover

$$(\pi, J^2, J_z, s, A, I^2, I_z)$$

### NPLQCD Phys.Rev. D87 (2013), 034506

				<b>-</b>		
Label	A	8	<u> </u>	$J^{\pi}$	Local SU(3) irreps	This work
N	1	0	1/2	$1/2^{+}$	8	8
Λ	1	-1	0	$1/2^{+}$	8	8
$\Sigma$	1	-1	1	$1/2^{+}$	8	8
Ξ	1	-2	1/2	$1/2^{+}$	8	8
d	2	0	0	1+	$\overline{10}$	$\overline{10}$
nn	2	0	1	$0^+$	27	27
$n\Lambda$	2	-1	1/2	$0^+$	27	27
$n\Lambda$	2	-1	1/2	1+	$8_A,  \overline{10}$	
$n\Sigma$	2	-1	3/2	$0^{+}$	27	27
$n\Sigma$	2	-1	3/2	1+	10	10
$n\Xi$	2	-2	0	1+	$8_A$	$8_A$
$n\Xi$	2	-2	1	1+	$8_A,  10,  \overline{10}$	
H	2	-2	0	$0^{+}$	1, <b>27</b>	1, <b>27</b>
<sup>3</sup> H, <sup>3</sup> He	3	0	1/2	$1/2^+$	35	35
$^3_\Lambda { m H}(1/2^+)$	3	-1	0	$1/2^{+}$	35	
$^3_\Lambda { m H}(3/2^+)$	3	-1	0	$3/2^{+}$	$\overline{10}$	$\overline{10}$
$^3_{\Lambda}{ m He},^3_{\Lambda}{ m \widetilde{H}},~nn\Lambda$	3	-1	1	$1/2^{+}$	$27,  \overline{35}$	$27, \overline{35}$
$^3_{\Sigma}\mathrm{He}$	3	-1	1	$3/2^{+}$	27	27
$^{4}\mathrm{He}$	4	0	0	0+	28	28
${}^4_{\Lambda}$ He, ${}^4_{\Lambda}$ H	4	-1	1/2	0+	$\overline{28}$	
$^{4}_{\Lambda\Lambda}$ He	4	-2	0	0+	$27,  \overline{28}$	27, <del>2</del> 8

#### NPLQCD Phys.Rev. D87 (2013), 034506

For example, for the A=3 system:

$$(48^3 \times 64)$$











#### NPLQCD Phys. Rev. D87 (2013) 3, 034506





Other works Remarkable progress up to A=4 systems



ress

Formalism developed that I did not cover:

♦ Including partial-wave mixing

- 1. M. Lüscher, Commun. Math. Phys. 105 (1986)
- 2. M. Lüscher, Nucl. Phys. B 354 (1991)
- 3. K. Rummukainen and S.A. Gotlieb, Nucl.Phys.B 450 (1995)
- 4. C.H. Kim, C.T.Sachrajda and S.R.Sharpe, Nucl.Phys.B 727 (2005)
- 5. T.Luu and M.J.Savage, PRD 83 (2011)
- 6. M.T.Hansen and S.R.Sharpe, PRD 86 (2012)
- 7. R.Briceño and Z.Davoudi, Phys.Rev. D88 (2013) 9, 094507
- 8. R.Briceño, Z.Davoudi and T.Luu, Phys.Rev. D88 (2013) 3, 034502
- 9. R.Briceño, Z.Davoudi, T.Luu and M.J.Savage, Phys.Rev. D88 (2013) 11, 114507
  - ♦ Including the electromagnetic interaction
  - 1. S. Drury et al., PoS LATTICE 2013 (2013) 268 [arXiv:1312.0477 [hep-lat]]
  - 2. S.R. Beane and M.J. Savage, arXiv:1407.4846 [hep-lat]
  - 3. K.U. Can et al., JHEP 1405 (2014) 125, [arXiv:1310.5915 [hep-lat]].

# Summary

High statistics Lattice QCD determinations allow us to extract the infinite volume binding energies of light nuclear and hypernuclear sytems.

We have found evidence of bound NN ( ${}^{1}S_{0}$  and  ${}^{3}S_{1}$ ),  $\Lambda\Lambda$  and  $\Xi\Xi$  ( ${}^{1}S_{0}$ ) systems at unphysical values of the quarks masses.

LQCD predictions for hypernuclear physics are possible: Scattering phase-shifts for the  $\,^1\!S_0$  and  $^3\!S_1$  n  $\Sigma^-$  channels

We require enough computational resources in order to undertake simulations at lighter quark masses and at multiple lattice spacings.

These calculations will allow us to perform reliable extrapolations to the physical mass point and to the continuum.

We have evolved very fast to the point where first principles calculations of light nuclei are possible. We need to secure computational resources in powerful supercomputers to continue with this program and provide some useful input to hypernuclear physics.

> Thank you for your attention